

AD-A221 546

DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED			1b. RESTRICTIVE MARKINGS		
2a. SECURITY CLASSIFICATION AUTHORITY			3. DISTRIBUTION / AVAILABILITY OF REPORT		
2b. DECLASSIFICATION / DOWNGRADING SCHEDULE					
4. PERFORMING ORGANIZATION REPORT NUMBER(S)			5. MONITORING ORGANIZATION REPORT NUMBER(S) AFOSR-TR-90-0476		
6a. NAME OF PERFORMING ORGANIZATION Gordon Research Conference		6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION AFOSR/NC		
6c. ADDRESS (City, State, and ZIP Code) University of Rhode Island Kingston, RI 18195			7b. ADDRESS (City, State, and ZIP Code) Building 410 Bolling AFB, DC 20332-6448		
8a. NAME OF FUNDING / SPONSORING ORGANIZATION AFOSR		8b. OFFICE SYMBOL (If applicable) NC	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER AFOSR-88-0193		
8c. ADDRESS (City, State, and ZIP Code) Building 410 Bolling AFB, DC 20332-6448			10. SOURCE OF FUNDING NUMBERS		
PROGRAM ELEMENT NO. 61102F		PROJECT NO. 2303	TASK NO. B2	WORK UNIT ACCESSION NO.	
11. TITLE (Include Security Classification) 1988 Gordon Research Conference on the Chemistry of Energetic Materials					
12. PERSONAL AUTHOR(S) C. B. Storm, and T. B. Brill					
13a. TYPE OF REPORT Final Report		13b. TIME COVERED FROM _____ TO _____		14. DATE OF REPORT (Year, Month, Day)	
15. PAGE COUNT 14					
16. SUPPLEMENTARY NOTATION					
17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)		
FIELD	GROUP	SUB-GROUP	ENERG- TR-90-0476		
19. ABSTRACT (Continue on reverse if necessary and identify by block number) A Gordon Research Conference on the Chemistry of Energetic Materials was held at the New Hampton School 27 June - 1 July 1988. There were 110 attendees. A broad range of topics were covered: reactions in energetic materials, modeling in reactive systems, equation of state, structural chemistry, thermal decomposition, new materials, spectroscopy in fast reactions, and chemistry at high pressure. There were 28 speakers who were recognized leaders in their technology areas. There were 40 poster papers on diverse topics.					
20. DISTRIBUTION / AVAILABILITY OF ABSTRACT <input type="checkbox"/> UNCLASSIFIED/UNLIMITED <input type="checkbox"/> SAME AS RPT. <input type="checkbox"/> DTIC USERS			21. ABSTRACT SECURITY CLASSIFICATION UNCLASSIFIED		
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**1988 GORDON RESEARCH CONFERENCE ON THE
CHEMISTRY OF ENERGETIC MATERIALS**

FINAL PROGRESS REPORT

GRANT AFOSR-88-0193

The Gordon research Conference on "The Chemistry of Energetic Materials" was held from June 27 to July 1, 1988 at the New Hampton School, New Hampton, New Hampshire. The conference had 110 participants, 13 per cent from foreign countries. There was a good mixture of scientists from universities, national laboratories, DoD laboratories, research institutes and private industry, including young scientists, graduate students, and postdoctoral associates as well as established scientists.

The program for the conference brought together research scientists working in several different areas, who share a common interest in the basic chemistry and physics of the performance and safety of energetic materials. The topics discussed included: Reactions in Energetic Materials, Modeling in Reactive Systems, Equation of State, Structural Chemistry, Thermal Decomposition, New Materials, Spectroscopy in Fast Reactions and Chemistry at High Pressure. The discussion following the talks was extensive and continued beyond the sessions into the afternoon and evening into the free time scheduled for the conferees. There was a poster session at which forty posters were presented. The posters were put up Tuesday afternoon and active discussion the the contents continued for the week.

Much of the discussion at the conference centered around the idea of what is the chemical speciation that takes place in the predetonation period, during the detonation and in a propellant burn. Central questions were addressed as to how these species can be detected spectroscopically, how they can be predicted from theoretical calculations, how they can be used in modeling the reaction and constructing kinetic models for the behavior of various energetic materials. Consideration was given to the role of molecular and crystal structure in predicting performance and understanding reactivity.

The general comments of the conferees was that it was a very successful Gordon Research Conference and a second conference has been requested for the summer of 1990. The 1990 conference will be Chaired by Professor Thomas B. Brill, Department of Chemistry, University of Delaware. Dr. Christos Capellos, US ARDEC, Dover, NJ was elected Vice Chairman of the 1990 conference.

Dist	Avail and/or Special
A-1	

GORDON RESEARCH CONFERENCE
CHEMISTRY OF ENERGETIC MATERIALS
NEW HAMPTON SCHOOL, NEW HAMPSHIRE
JUNE 27 - JULY 1, 1988

C. B. Storm, Chairman

T. B. Brill, Vice Chairman

PROGRAM SCHEDULE

Monday, June 27

7:45 AM BREAKFAST

8:30-8:40 AM, Welcome and organizational comments, C. B. Storm.

SESSION 1. REACTIONS IN ENERGETIC MATERIALS, J. P. RITCHIE, DIS. LDR.

**8:40-9:15 AM, J. P. RITCHIE, THEORETICAL CALCULATIONS OF THE
STRUCTURE, ENERGY AND REACTIONS OF EXPLOSIVES.**

9:15-9:25 DISCUSSION

**9:25-10:00 J. R. MURDOCH, REACTIVITY AND THERMODYNAMICS OF
ENERGETIC MATERIALS. PREDICTIONS FROM
EXPERIMENTAL DATA.**

10:00-10:10 DISCUSSION

10:10-10:30 COFFEE BREAK AND GROUP PHOTOGRAPH

**10:30-11:05 C. F. MELIUS, REACTION MECHANISMS IN THE IGNITION
AND COMBUSTION OF NITRAMINES.**

11:05-11:15 DISCUSSION

11:15-11:50 P. GRAY, THERMAL FEEDBACK AND INSTABILITIES.

11:50-12:10 DISCUSSION

12:30 LUNCH

6:00 PM DINNER

SESSION 2. MODELING IN REACTIVE SYSTEMS, D. S. STEWART, DIS. LDR.

**7:30-8:05 PM, J. B. BDZIL, STATE-DEPENDENT REACTION RATES: THEIR
ROLE IN DETERMINING THE STRUCTURE OF THE
DETONATION REACTION ZONE.**

8:05-8:15 DISCUSSION

8:15-8:45 D. S. STEWART, DETONATION STABILITY.

8:45-8:55 DISCUSSION

8:55-9:10 BREAK

**9:10-9:45 D. KASSOY, A COMPARISON BETWEEN DIFFUSIVE AND
NONDIFFUSIVE THERMAL EXPLOSION PHENOMENA.**

9:45-9:55 DISCUSSION

TUESDAY, JUNE 28

7:45 AM BREAKFAST

SESSION 3. EQUATION OF STATE, J. D. JOHNSON, DISC. LDR.

8:30-9:10 AM F. H. REE, MULTIPHASE MIXTURE EOS UNDER REACTIVE
AND NONREACTIVE ENVIRONMENTS.
9:10-9:20 DISCUSSION
9:20-10:00 W. BYERS BROWN, THE EFFECTS OF CHEMISTRY AND
PHASE CHANGES ON THE IDEAL DETONATION STATE.
10:00-10:10 DISCUSSION.
10:10-10:30 COFFEE BREAK
10:30-11:10 M. S. SHAW, DENSE FLUID EQUATION OF STATE: THEORY
AND SIMULATIONS.
11:10-11:20 DISCUSSION
11:20-12:00 J. D. JOHNSON, CARBON COAGULATIONS IN DETONATIONS.
12:00-12:10 Discussion
12:30 LUNCH

4:30-6:00 PM POSTER SESSION

6:00 DINNER

SESSION 4. STRUCTURAL CHEMISTRY, H. AMMON, DISC. LDR.

7:30-8:15 PM J. HOLDEN, PREDICTION OF CRYSTAL STRUCTURE FROM
MOLECULAR CONFORMATION.
8:15-8:25 DISCUSSION.
8:25-8:40 BREAK
8:40-9:25 C. LOWE-MA, DOES THE CRYSTAL STRUCTURE PLAY A
ROLE IN AN ENERGETIC MATERIALS PROPERTIES?
9:25-9:35 DISCUSSION

WEDNESDAY, JUNE 29
7:45 AM BREAKFAST

SESSION 5, THERMAL DECOMPOSITION, T. B. BRILL, DISC. LDR.

8:30-9:10 AM T. B. BRILL, FAST THERMAL DECOMPOSITION CHEMISTRY.
9:10-9:20 DISCUSSION
9:20-10:00 A. C. ECKBRETH, NEW CONCEPTS FOR CARS DIAGNOSTICS
OF SOLID PROPELLANT COMBUSTION.
10:10-10:10 DISCUSSION
10:10-10:30 COFFEE BREAK
10:30-11:10 X. ZHAO, CONCERTED DISSOCIATION IN RING COMPOUNDS.
11:10-11:20 DISCUSSION
11:20-12:00 R. BEHRENS, INVESTIGATIONS OF HMX AND RDX THERMAL
DECOMPOSITIONS WITH SIMULTANEOUS
THERMOGRAVIMETRIC MODULATED MOLECULAR BEAM
MASS SPECTROMETRY ANALYSIS.
12:00-12:10 DISCUSSION
12:30 LUNCH

4:30-6:00 PM BUSINESS MEETING.

6:00 DINNER

SESSION 6, NEW MATERIALS, D. McMillen, DISC. LDR.

7:30-8:05 PM A. T. NIELSEN, SYNTHESIS OF CAGED NITRAMINE COMPOUNDS
8:05-8:15 DISCUSSION.
8:15-8:50 P. E. EATON, NEW WORK WITH THE CUBANE SYSTEM.
8:50-9:00 DISCUSSION
9:00-9:15 BREAK
9:15-9:50 R. SCHMITT, HYPOTHETICAL STRUCTURES FOR EXPLOSIVES AND PROPELLANTS.
9:50-10:00 DISCUSSION

THURSDAY, JUNE 30
7:45 AM BREAKFAST

SESSION 7, SPECTROSCOPY IN FAST REACTIONS, A. M. RENLUND, DISC. LDR.

8:30-9:10 AM C. WITTIG, PHOTOINITIATED REACTIONS IN UNIQUE ENVIRONMENTS.
9:10-9:20 DISCUSSION
9:20-10:00 W. TROTT, REAL-TIME SPECTROSCOPIC STUDIES OF SHOCKED ENERGETIC MATERIALS.
10:00-10:10 DISCUSSION
10:10-10:30 COFFEE BREAK
10:30-11:10 S. DUFORT, THE USE OF TIME RESOLVED SPECTROSCOPIES IN THE STUDY OF THE INITIATION OF EXPLOSIVES AT THE MOLECULAR LEVEL.
11:10-11:20 DISCUSSION
11:20-12:00 K. EISENTHAL, LASER STUDIES OF ULTRA-FAST PROCESSES IN LIQUIDS.
12:00-12:10 DISCUSSION
12:30 LUNCH
6:00 PM DINNER

SESSION 8, 7:30 PM, W. C. DAVIS, OUTSTANDING PROBLEMS IN DETONATION SCIENCE; FOLLOWED BY A PANEL DISCUSSION: G. A. LEIPER, R. S. MILLER, A. M. RENLUND.

FRIDAY, JULY 1
7:45 AM BREAKFAST

SESSION 9, CHEMISTRY AT HIGH PRESSURE, S. TREVINO, DISC. LDR.

8:30-9:10 AM P. MILLER, EFFECTS OF PRESSURE AND TEMPERATURE ON THE KINETICS AND CHEMICAL REACTIVITY OF NITRAMINE EXPLOSIVES.

9:10-9:20 DISCUSSION

9:20-10:00 M. NICOL, REACTIONS AND STRUCTURES OF SOME UNSATURATED H-C-N-O SOLIDS AT HIGH STATIC AND DYNAMIC PRESSURES.

10:00-10:10 DISCUSSION

10:10-10:30 COFFEE BREAK

10:30-11:10 S. AGNEW, HIGH PRESSURE REACTIONS OF ENERGETIC MATERIALS: NITROMETHANE AND NITRIC OXIDE.

11:10-11:20 DISCUSSION

LUNCH & DEPARTURE.

GORDON RESEARCH CONFERENCE
CHEMISTRY OF ENERGETIC MATERIALS
NEW HAMPTON SCHOOL, NEW HAMPSHIRE
JUNE 27 - JULY 1, 1988

POSTER SESSION
TUESDAY, JUNE 28, 1988; 4:30-6:00 PM

H. L. AMMON AND R. W. ARMSTRONG, MODELING STUDIES OF RDX AND HMX CRYSTAL DEFORMATIONS.

R. C. ARMSTRONG, CHEMICAL AND HYDRODYNAMIC CONTRIBUTIONS TO LIQUID MONOPROPELLANT STABILITY.

A. BASHIR-HASHEMI, NEW DEVELOPMENTS IN CUBANE CHEMISTRY - PHENYL CUBANES.

B. C. BEARD AND J. SHARMA, RADIATION SENSITIVITY AND DECOMPOSITION OF NTC

N. BLAIS, THE FREE EXPANSION OF DETONATION PRODUCTS IN VACUUM.

P. BRUSH AND T. B. BRILL, FAST HEAT AND HOLD DECOMPOSITION OF HMX AND RD

F. BUGAUT, THERMODYNAMICS OF DENSE FLUID NITROGEN BY MONTE CARLO SIMULATION.

R. J. BUTCHER, A. OKONKOW, N. S. ROWAN-FORDON AND A. NGUYEN-PHO, FAVORABLE ELECTROPHILIC SUBSTITUTION IN METAL ION COORDINATED HETEROCYCLES.

R. S. DAMAVARAPPU AND S. IYER, SYNTHETIC DESIGNS TOWARDS POLYNITROPOLYHEDRANES.

L. R. DOSSER, LASER ILLUMINATED HIGH SPEED PHOTOGRAPHY OF ENERGETIC MATERIALS.

L. R. DOSSER, LASER IGNITION OF ENERGETIC MATERIALS.

C. H. DOUGLAS AND J. K. RICE, NASCENT BH DISTRIBUTIONS FROM THE PHOTODISSOCIATION OF BH₃CO AT 193 nm.

W. ELBAN, P. J. COYNE, JR., R. W. ARMSTRONG, H. W. SANDUSKY, B. C. GLANCY, AND D. W. CARLSON, BIG POINTS FROM SMALL IMPRESSIONS IN AMMONIUM PERCHLORATE.

D. W. FIRSICH, POLYMORPHISM IN HEXANITROAZOBENZENE.

M. F. Foltz and C. B. Moore, PHOTOFRAGMENT DYNAMICS OF FORMALDEHYDE.

M. J. B. GREEN, M. J. PILLING AND S. H. ROBERTSON, DIFFUSION AND DETONATION.

J. A. HOLY AND T. C. GIRMANN, THE EFFECTS OF PRESSURE ON THE LASER INITIATION OF $TiH_x/KClO_4$ AND OTHER PYROTECHNICS.

S. R. JAIN, PREIGNITION REACTIONS IN HYPERGOLIC SYSTEMS.

K. JAYASURIYA AND O. SANDUS, EFFECT OF SUBSTITUENT GROUPS ON STRAIN ENERGY.

J. J. KAUFMAN, AB-INITIO MRD-CI CALCULATIONS FOR BREAKING A CHEMICAL BOND IN A MOLECULE IN A CRYSTAL OR OTHER SOLID ENVIRONMENT: NITROMETHANE.

S. Lambrakos, M. Peyrard and E. S. Oran, ANALYSIS OF MICROSCOPIC STRUCTURE OF DETONATIONS IN ENERGETIC SOLIDS.

J. F. LIEBMAN, J. S. CHICKOS, D. G. HESSE S. Y. PANSIN AND K. A. GEORGIU, ESTIMATION OF HEATS OF VAPORIZATION AND SUBLIMATION OF ORGANIC COMPOUNDS.

W. L. LUKASAVAGE, A. BOHON, J. ALSTER AND S. NICOLICH, ISOTHERMAL PREPARATION OF 3,7-DIACETYL-1,3,5,7-TETRAAZABICYCLO-3,3,1-NONANE (DAPT).

A. P. MARCHAND, SYNTHESIS OF NOVEL POLYNITROPOLYCYCLIC COMPOUNDS: A NEW CLASS OF ENERGETIC MATERIALS.

R. W. MILLAR, NITRATION OF STRAINED RING COMPOUNDS.

R. MOWREY, THEORETICAL STUDY OF METHYLENENITRAMINE DECOMPOSITION.

S. ODIOT, DISSIPATION ENERGY AND DETONATION WAVE IN AN ENERGETIC MOLECULAR CRYSTAL.

V. R. PAI VERNEKER, ROLE OF CRYSTAL DEFECTS IN THE THERMAL REACTIVITY OF ENERGETIC MATERIALS.

P. PAPAGIANNAKOPOULOS AND C. CAPELLOS, KrF PHOTODECOMPOSITION OF TETRANITROMETHANE.

J. K. RICE, N. J. CALDWELL AND H. H. NELSON, REACTIONS OF BH_3 .

R. C. Sausa, ELECTRONICALLY EXCITED SPECIES GENERATED BY EXCIMER LASER EXCITATION OF DIMETHYLNITRAMINE.

M. A. SCHROEDER, THERMAL DECOMPOSITION OF CATALYZED AND UNCATALYZED HMX PROPELLANT FORMULATIONS.

J. SHARMA, C. S. COFFEY, T. P. LIPPARD AND J. FORBES, CHEMICAL REACTIONS IN EXPLOSIVES PRECEDING IGNITION.

J. E. SHEPHERD, REACTION ZONE STRUCTURE IN GASEOUS MOLECULAR EXPLOSIVES.

G. P. SOLLOTT, POLYSUBSTITUTED ADAMANTANES EN ROUTE TO POLYNITROTRICYCLODECANES (ADAMANTANES), TRICYCLOOCTANES AND TRICYCLOHEXANES.

R. J. Spear, PARTICLE SIZE EFFECTS ON SHOCK SENSITIVITY OF RDX.

P. STEWART, J. B. JEFFRIES, J-M. ZELWEGGER, D. F. McMILLEN AND D. M. GOLDEN, LASER-POWERED HOMOGENEOUS PYROLYSIS OF DIMETHYLNITRAMINE DECOMPOSITION. GC/MS AND MOLECULAR BEAM/MS STUDIES.

C. B. STORM, ^1H - ^2H EXCHANGE IN NITROMETHANE.

J. H. STUFFLEBEAM, CARS APPLICATIONS TO SOLID PROPELLANT COMBUSTION.

H-t. WANG, C. Y. LIN AND M. C. LIN, THERMAL DECOMPOSITION OF NO_2 AND THE CHEMICAL KINETICS OF THE $\text{HCHO} + \text{NO}_2$ REACTION.

C-S. YOO, CHEMISTRY ON SHOCK COMPRESSED ORGANIC MOLECULES.

W. W. ZAJAC, TRANSFORMATION OF NITROGEN CONTAINING FUNCTIONAL GROUPS INTO NITRO GROUPS.

GORDON RESEARCH CONFERENCES
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New Hampton School
June 27 - July 1, 1988

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